

1-Methyl-2-propylbenzene
1074-17-5 | DTXSID4061466

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -56.4 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 7.16e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Diethylbenzene

Measured: -42.8

Predicted: -56.4

Image not found

1-Methyl-2-propylbenzene

Measured: -60.3

Predicted: -56.4

Image not found

p-Propyltoluene

Measured: -63.6

Predicted: -56.4

Image not found

o-Diethylbenzene

Measured: -31.2

Predicted: -56.4

Image not found

1,3-Diethylbenzene

Measured: -83.9

Predicted: -56.4